=> file caplus

FILE 'CAPLUS' ENTERED AT 14:03:15 ON 15 FEB 2002
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FILE COVERS 1907 - 15 Feb 2002 VOL 136 ISS 8
FILE LAST UPDATED: 14 Feb 2002 (20020214/ED)

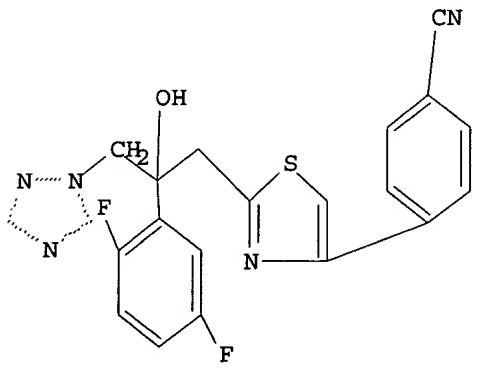
This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the CAS files between 12/27/01 and 1/23/02. As of 1/23/02, the situation has been resolved. Searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator executed between 12/27/01 and 1/23/02 may be incomplete. See the NEWS message on this topic for more information.

=> d que

L1 STR



Structure attributes must be viewed using STN Express query preparation.
L3 87 SEA FILE=REGISTRY SSS FUL L1
L4 2 SEA FILE=CAPLUS L3

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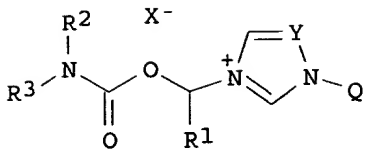
L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:338523 CAPLUS
DOCUMENT NUMBER: 134:353309
TITLE: Synthesis and formulation of N-substituted carbamoyloxyalkyl-azolium derivatives and their use as antifungal agents
INVENTOR(S): Fukuda, Hiroshi; Hayase, Tadakatsu; Mizuguchi, Eisaku; Shimma, Nobuo; Ohwada, Jun; Oikawa, Nobuhiro; Sakaitani, Masahiro; Tsukazaki, Masao; Umeda, Isao
PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.
SOURCE: PCT Int. Appl., 83 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001032652	A2	20010510	WO 2000-EP10524	20001025

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: EP 1999-121694 A 19991102
OTHER SOURCE(S): MARPAT 134:353309
GI



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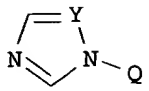

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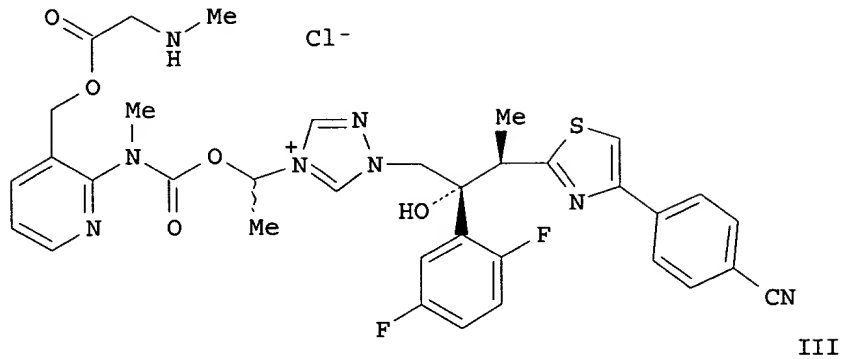

III

AB The synthesis and use of N-substituted carbamoyloxyalkyl-azolium derivs. of general formula I are claimed as antifungal agents [wherein Q is a group of an antifungal azole of formula II; Y is N or CH; R1 is H or alkyl; R2 is H, alkyl, alkylcarbonyloxyalkyl, alkoxycarbonyl, alkylcarbonyl, mono- or dialkylaminoalkylcarbonyloxyalkyl; R3 is alkylaminoalkyl, alkylcarbonyl(oxy)alkyl, optionally substituted Ph, pyridin-2-yl, etc. or the group R2R3N may form an optionally substituted pyrrolidine, pyrrolidone or piperidine; X- is a pharmaceutically acceptable anion]. For instance, the synthesis of III occurs via the alkylation of 1-[(2R,3R)-3-[4-(4-cyanophenyl)thiazol-2-yl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-[1,2,4]-triazole (IV, prepd. in 8 steps) with N-methyl-N-(3-[((N-tert-butoxycarbonyl-N-methylamino)acetoxy)methyl)pyridin-2-yl]carbamic acid 1-chloroethyl ester (prepd. from 2-chloronicotinic acid) in CH3CN with NaI at 45-50.degree.C for 15 h. Deprotection of the resulting salt with HCl led to the isolation of III as the dihydrochloride salt. Soly. of the invention compds. was detd. in distd. water and said to be greater than known antimycotic azoles of formula II. In particular, III soly. in water and physiol. saline was >1000 mg/mL. Representative compds. I were incubated with human plasma (10 .mu.g/mL) at 37.degree.C up to 2 h resulting in degrdn. to common metabolite IV in <6 min (6 exs.). Antifungal activity of compds. I and Fluconazole and Itraconazole was detd. in male Fisher rats infected with C. albicans or A. fumigatus administered i.v. and p.o. ED50 (.mu.mol/kg) for III was 2.8 (i.v.) and 7 (p.o.) against C. albicans UTHS93-2067 vs. 8.1 for Fluconazole and 4.2 for Itraconazole (both p.o.). A description of an i.m., gelatin capsule and tablet formulation are provided as well as detailed HPLC anal. data for representative compds. Azolium salts I are for the prophylaxis and/or treatment of fungal infections.

IT **338990-72-0P 338990-80-0P 338990-81-1P 338990-82-2P 338990-84-4P 338990-94-6P 338990-99-1P 338991-04-1P 338991-05-2P**

338991-10-9P 339307-64-1P
RL: BAC (Biological activity or effector, except adverse); IMF (Industrial
manufacture); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of N-substituted carbamoyloxyalkyl-azolium derivs. and their
use as antifungal agents)

IT 22916-47-8DP, Miconazole, derivs. of 65277-42-1DP, Ketoconazole, derivs.
of 84625-61-6DP, Itraconazole, derivs. of 136067-84-0DP, derivs. of 136657-97-1DP, derivs. of 149715-95-7DP, derivs. of 151856-47-2DP, derivs. of 155432-64-7DP, derivs. of 182760-06-1DP, derivs. of 213381-02-3DP, derivs. of **241479-66-3DP**, derivs. of **241479-67-4DP**, derivs. of 241479-68-5DP, derivs. of **338990-73-1P 338990-74-2P 338990-75-3P 338990-76-4P 338990-77-5P 338990-78-6P 338990-79-7P 338990-83-3P 338990-85-5P 338990-86-6P 338990-87-7P 338990-88-8P 338990-89-9P 338990-90-2P 338991-91-3P 338990-92-4P 338990-93-5P 338990-95-7P 338990-96-8P 338990-97-9P 338990-98-0P 338991-00-7P 338991-01-8P 338991-02-9P 338991-03-0P 338991-06-3P 338991-07-4P 338991-08-5P 338991-09-6P 338991-11-0P 338991-12-1P 338991-13-2P 338991-14-3P** 338991-15-4P 338991-16-5P 338991-17-6P 338991-18-7P 338991-19-8P 338991-20-1P 338991-21-2P 338991-22-3P 338991-23-4P 338991-25-6P 338991-27-8P 338991-29-0P 338991-30-3P 338991-31-4P 338991-32-5P 338991-33-6P 338991-34-7P 338991-35-8P 338991-36-9P 338991-37-0P 338991-38-1P 338991-39-2P 338991-40-5P 338991-41-6P 338991-42-7P 338991-43-8P 338991-44-9P 338991-45-0P 338991-46-1P 338991-47-2P **338991-48-3P 338991-49-4P 338991-50-7P** 338991-51-8P 338991-52-9P 338991-53-0P
RL: BAC (Biological activity or effector, except adverse); IMF (Industrial
manufacture); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of N-substituted carbamoyloxyalkyl-azolium derivs. and their
use as antifungal agents)

IT 2258-42-6P, Acetic formic anhydride 14667-47-1P, Methyl 2-aminonicotinate 29055-08-1P 32399-12-5P, 2-(N-Methylamino)-3-hydroxymethylpyridine 49609-84-9P, 2-Chloronicotinoyl chloride 122734-34-3P 186353-05-9P, Chloromethyl N-Methyl-N-(phenyl)carbamate 232951-83-6P, tert-Butyl 2-chloronicotinate 338990-20-8P, Chloromethyl N-Methyl-N-(2-(acetoxymethyl))phenylcarbamate 338990-21-9P, 1-Chloroethyl N-Methyl-N-(3-(acetoxymethyl)pyridin-2-yl)carbamate 338990-22-0P, 1-Chloroethyl N-Acetyl-N-methylcarbamate 338990-23-1P, 2(S)-Acetoxymethyl-1-(chloromethyloxycarbonyl)pyrrolidine 338990-24-2P, Chloromethyl N-Methyl-N-(2-acetoxyethyl)carbamate 338990-25-3P, N-Methyl-N-(3-acetoxypropyl)carbamic acid chloromethyl ester 338990-26-4P, N-(2-Methylphenyl)-N-(2-acetoxyethyl)carbamic acid chloromethyl ester 338990-27-5P 338990-28-6P 338990-29-7P 338990-30-0P, N-Methyl-N-(2-((N-(tert-butoxycarbonyl)-N-(methyl)amino)methyl)phenyl)carbamic acid 1-chloroethyl ester 338990-31-1P, N-Methyl-N-(3-[((N-tert-butoxycarbonyl-N-methylamino)acetoxy)methyl)pyridin-2-yl]carbamic acid 1-chloroethyl ester

338990-32-2P 338990-33-3P 338990-34-4P 338990-35-5P 338990-36-6P
338990-37-7P 338990-38-8P 338990-39-9P 338990-40-2P 338990-41-3P
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338990-47-9P 338990-48-0P 338990-49-1P 338990-50-4P 338990-51-5P
338990-52-6P 338990-53-7P 338990-54-8P 338990-55-9P 338990-56-0P
338990-57-1P 338990-58-2P 338990-59-3P 338990-60-6P 338990-61-7P
338990-62-8P 338990-63-9P 338990-64-0P
338990-65-1P 338990-66-2P, Isopropyl-(2-nitrobenzyl)carbamic acid tert-butyl ester 338990-67-3P, Isopropyl(2-Aminobenzyl)carbamic acid tert-butyl ester 338990-68-4P, Isopropyl-(2-methylaminobenzyl)carbamic acid tert-butyl ester 338990-70-8P, tert-Butyl 2-(N-methylamino)nicotinate 338990-71-9P, Methyl 2-(N-formylamino)nicotinate 338991-54-1P, N-Isopropyl-2-nitrobenzylamine 338991-55-2P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of N-substituted carbamoyloxyalkyl-azolium derivs. and their use as antifungal agents)

IT **241479-67-4P**, 1-[(2R,3R)-3-[4-(4-Cyanophenyl)thiazol-2-yl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-[1,2,4]-triazole
RL: MFM (Metabolic formation); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation)
(synthesis of N-substituted carbamoyloxyalkyl-azolium derivs. and their use as antifungal agents)

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:576927 CAPLUS
DOCUMENT NUMBER: 131:199700
TITLE: Preparation of 3-[4-(4-cyanophenyl)thiazol-2-yl)]-1-(1H-1,2,4-triazol-1-yl)-butan-2-ols as antifungals.
INVENTOR(S): Hayase, Tadakatsu; Ichihara, Shigeyasu; Isshiki, Yoshiaki; Liu, Pingli; Ohwada, Jun; Sakai, Toshiya; Shimma, Nobuo; Tsukazaki, Masao; Umeda, Isao; Yamazaki, Toshikazu
PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.
SOURCE: PCT Int. Appl., 68 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9945008	A1	19990910	WO 1999-EP1327	19990301
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RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9929313	A1	19990920	AU 1999-29313	19990301

US 6300353 B1 20011009 US 1999-263027 19990305
PRIORITY APPLN. INFO.: EP 1998-104036 A 19980306
EP 1998-123310 A 19981208
EP 1999-101360 A 19990126
WO 1999-EP1327 W 19990301
OTHER SOURCE(S): MARPAT 131:199700
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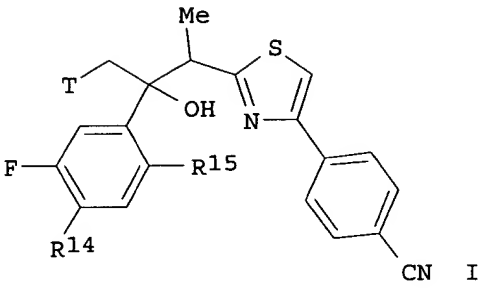

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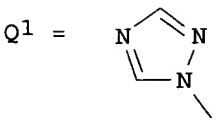

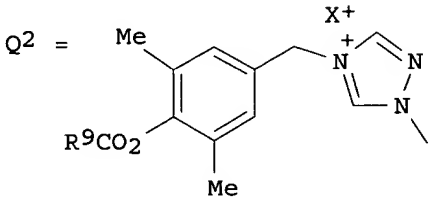

AB Title compds. [I; R14, R15 = H, F; T = Q1, Q2; R9 = pyrrolidinyl, ANHB; A = H, alkyl; B = alkylene, CH2CONHCH2, (CH2)3CH(NH2); X = pharmaceutically acceptable anion], were prepd. Thus, 4-[2-[(1R,2R)-2-(2,5-difluorophenyl)-2-hydroxy-1-methyl-3-(1,2,4-triazol-1-yl)propyl]thiazol-4-yl]benzonitrile (prepn. given) and 4-tert-butoxycarbonylmethylaminoacetoxy-3,5-dimethylbenzyl bromide were refluxed 15 h in MeCN; the product was stirred with aq. HCl in EtOAc to give 1-[(2R,3R)-3-[4-(4-cyanophenyl)thiazol-2-yl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-4-(3,5-dimethyl-4-methylaminoacetoxybenzyl)-1H-1,2,4-triazol-4-ium bromide (II). II inhibited candidiasis in rats with ED50 = 5.3 .mu.mol/kg. Drug formulations contg. II are given.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

IT **241479-18-5P 241479-20-9P 241479-21-0P**
241479-23-2P 241479-24-3P 241479-26-5P **241479-27-6P**
241479-29-8P 241479-30-1P 241479-32-3P
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241479-62-9P **241479-63-0P** **241479-64-1P** 241479-65-2P
241479-66-3P **241479-67-4P** 241479-68-5P 241479-88-9P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of cyanophenylthiazolyltriazolylbutanols as antifungals)

IT 20099-89-2P, 2-Bromo-4'-cyanoacetophenone 135206-87-0P 135270-08-5P
241479-69-6P 241479-70-9P 241479-71-0P 241479-72-1P 241479-73-2P
241479-74-3P 241479-75-4P 241479-76-5P 241479-77-6P 241479-78-7P
241479-79-8P 241479-80-1P 241479-81-2P 241479-82-3P
241479-83-4P 241479-84-5P 241479-85-6P 241479-86-7P
241479-87-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of cyanophenylthiazolyltriazolylbutanols as antifungals)

=> file uspatfull

FILE 'USPATFULL' ENTERED AT 14:04:26 ON 15 FEB 2002
CA INDEXING COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 14 Feb 2002 (20020214/PD)
FILE LAST UPDATED: 14 Feb 2002 (20020214/ED)
HIGHEST GRANTED PATENT NUMBER: US6330719
HIGHEST APPLICATION PUBLICATION NUMBER: US2002019999
CA INDEXING IS CURRENT THROUGH 14 Feb 2002 (20020214/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 14 Feb 2002 (20020214/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Dec 2001
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Dec 2001

>>> Page images are available for patents from 1/1/1998. Patents <<<
>>> and applications are typically loaded on the day of publication.<<<
>>> Page images are available for display by the following day. <<<
>>> Image data for the /FA field are available the following update.<<<

>>> Complete CA file indexing for chemical patents (or equivalents) <<<
>>> is included in file records. A thesaurus is available for the <<<
>>> USPTO Manual of Classifications in the /NCL, /INCL, and /RPCL <<<
>>> fields. This thesaurus includes catchword terms from the <<<
>>> USPTO/MOC subject headings and subheadings. Thesauri are also <<<
>>> available for the WIPO International Patent Classification <<<
>>> (IPC) Manuals, editions 1-6, in the /IC1, /IC2, /IC3, /IC4, <<<
>>> /IC5, and /IC (/IC6) fields, respectively. The thesauri in <<<
>>> the /IC5 and /IC fields include the corresponding catchword <<<
>>> terms from the IPC subject headings and subheadings. <<<

This file contains CAS Registry Numbers for easy and accurate substance identification.

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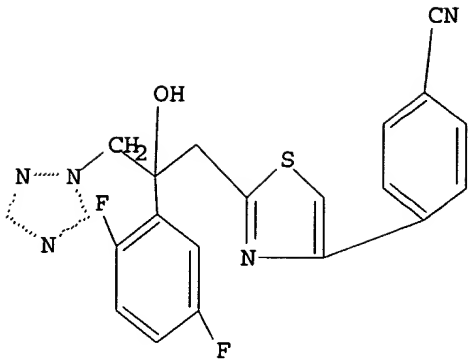
L1 STR



Structure attributes must be viewed using STN Express query preparation.
L3 87 SEA FILE=REGISTRY SSS FUL L1
L5 1 SEA FILE=USPATFULL L3

=> d l5 ibib abs hitstr

L5 ANSWER 1 OF 1 USPATFULL
ACCESSION NUMBER: 2001:173607 USPATFULL
TITLE: Azoles for treatment of fungal infections
INVENTOR(S): Hayase, Tadakatsu, Chigasaki, Japan
Ichihara, Shigeyasu, Kawasaki, Japan
Isshiki, Yoshiaki, Chigasaki, Japan
Liu, Pingli, Fujisawa, Japan
Ohwada, Jun, Kamakura, Japan
Sakai, Toshiya, Fujisawa, Japan
Shimma, Nobuo, Chigasaki, Japan
Tsukazaki, Masao, Fujisawa, Japan
Umeda, Isao, Yokohama, Japan
Yamazaki, Toshikazu, Kamakura, Japan
PATENT ASSIGNEE(S): Basilea Pharmaceutica AG, a Swiss Company, Basel, Switzerland (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6300353	B1	20011009
APPLICATION INFO.:	US 1999-263027		19990305 (9)

	NUMBER	DATE
PRIORITY INFORMATION:	EP 1998-104036	19980306
	EP 1998-123310	19981208
	EP 1999-101360	19990126

DOCUMENT TYPE: Utility
FILE SEGMENT: GRANTED
PRIMARY EXAMINER: Gerstl, Robert
LEGAL REPRESENTATIVE: Johnston, George W., Tramaloni, Dennis P.
NUMBER OF CLAIMS: 37
EXEMPLARY CLAIM: 1
LINE COUNT: 1686
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Azole derivatives of the formula I ##STR1##

wherein

R.sup.14, R.sup.15 are each independently hydrogen or fluorine,

T is a group of the formula: ##STR2##

wherein

R.sup.9 is pyrrolidinyl or a group A--NH--B--,

A is hydrogen or straight-chain or branched C.sub.1 -C.sub.5 alkyl;

B is straight-chain or branched C.sub.1 -C.sub.4 alkylene, --CH.sub.2 --CONH--CH.sub.2 or --CH.sub.2 CH.sub.2 CH.sub.2 --CH(NH.sub.2); and

X.sup.- is a pharmaceutically acceptable anion;

and pharmaceutically acceptable salts of said compounds, and hydrates and solvates of the compounds of formula I and the salts thereof can be used in the production of medicaments for treating fungal infections and

mycoses.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT **241479-18-5P 241479-20-9P 241479-21-0P**
241479-23-2P 241479-27-6P 241479-29-8P
241479-30-1P 241479-32-3P 241479-36-7P
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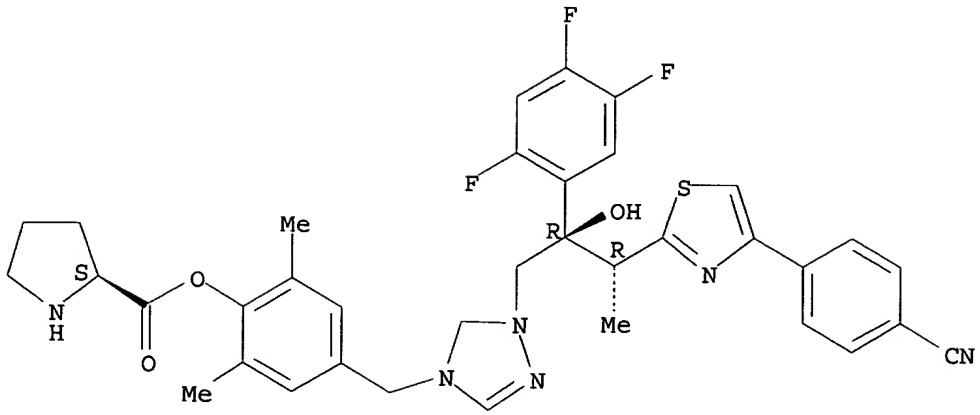
241479-61-8P 241479-63-0P 241479-64-1P
241479-66-3P 241479-67-4P
(prepn. of cyanophenylthiazolyltriazolylbutanols as antifungals)

RN 241479-18-5 USPATFULL

CN L-Proline, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-hydroxy-2-(2,4,5-trifluorophenyl)butyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Br^-

FRAGMENT DIAGRAM IS INCOMPLETE

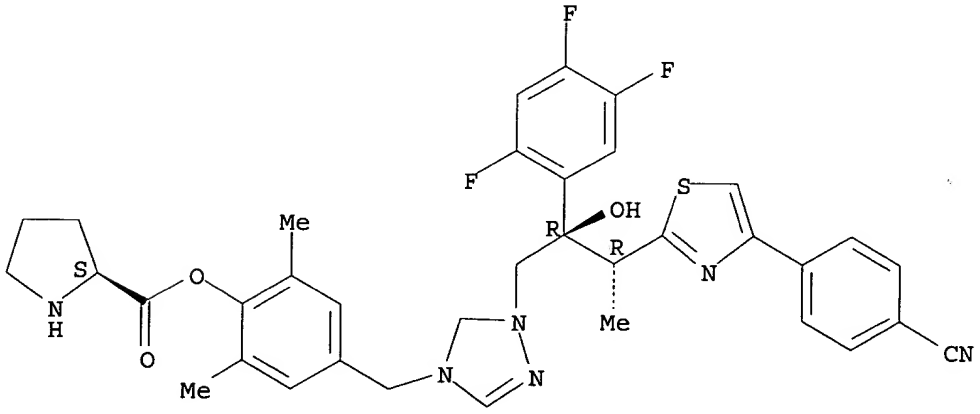
RN 241479-20-9 USPATFULL

CN L-Proline, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-hydroxy-2-(2,4,5-trifluorophenyl)butyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 241479-19-6
CMF C36 H34 F3 N6 O3 S

Absolute stereochemistry.

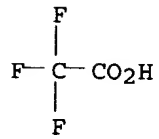


FRAGMENT DIAGRAM IS INCOMPLETE

CM 2

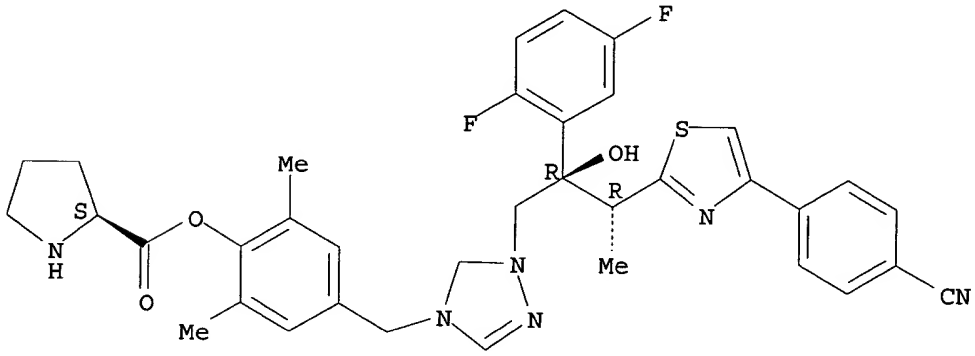
CRN 76-05-1

CMF C2 H F3 O2



RN 241479-21-0 USPATFULL
CN L-Proline, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Br^-

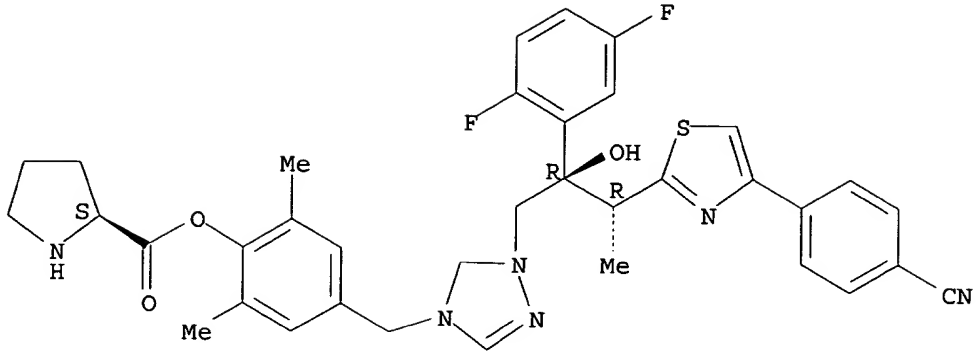
FRAGMENT DIAGRAM IS INCOMPLETE

RN 241479-23-2 USPATFULL
CN L-Proline, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 241479-22-1
CMF C36 H35 F2 N6 O3 S

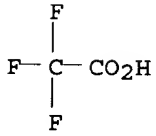
Absolute stereochemistry.



FRAGMENT DIAGRAM IS INCOMPLETE

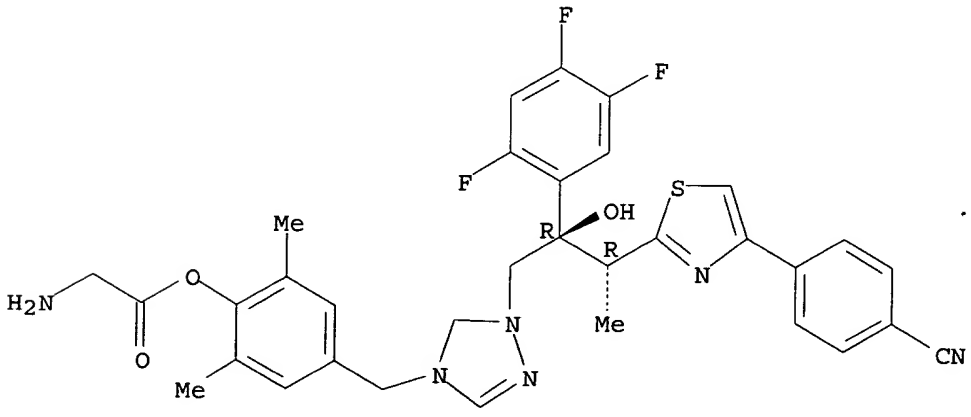
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 241479-27-6 USPATFULL
CN Glycine, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-hydroxy-2-(2,4,5-trifluorophenyl)butyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Br^-

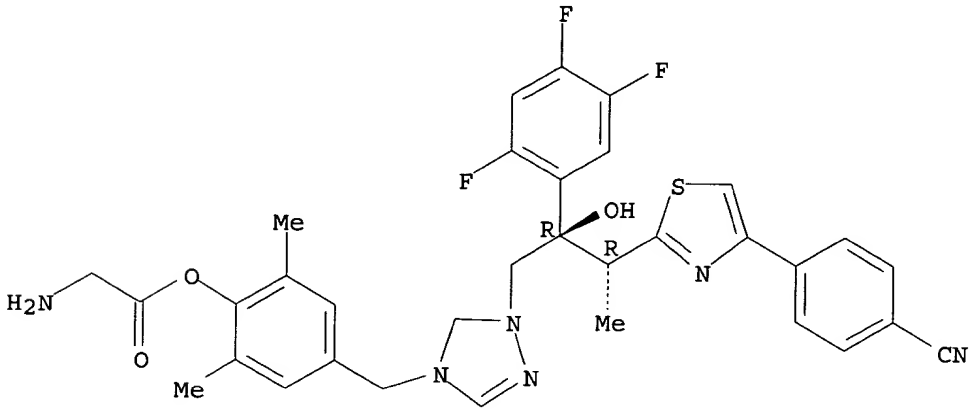
FRAGMENT DIAGRAM IS INCOMPLETE

RN 241479-29-8 USPATFULL
CN Glycine, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-hydroxy-2-(2,4,5-trifluorophenyl)butyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 241479-28-7
CMF C33 H30 F3 N6 O3 S

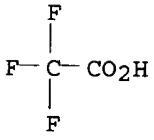
Absolute stereochemistry.



FRAGMENT DIAGRAM IS INCOMPLETE

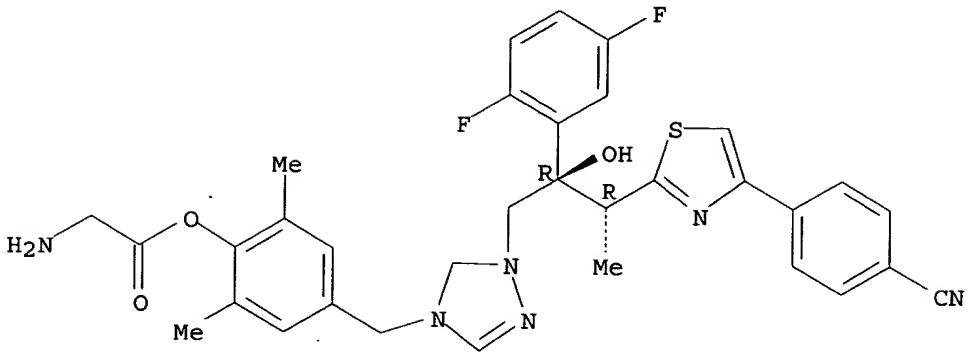
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 241479-30-1 USPATFULL
CN Glycine, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Br^-

FRAGMENT DIAGRAM IS INCOMPLETE

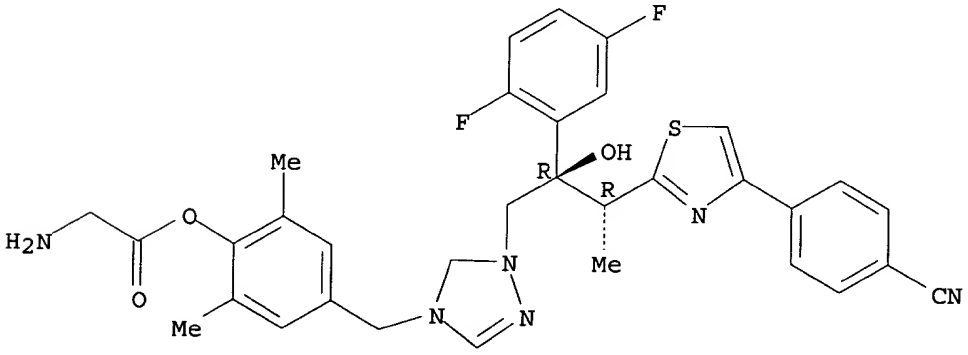
RN 241479-32-3 USPATFULL

CN Glycine, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 241479-31-2
CMF C33 H31 F2 N6 O3 S

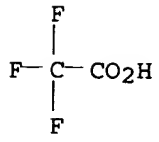
Absolute stereochemistry.



FRAGMENT DIAGRAM IS INCOMPLETE

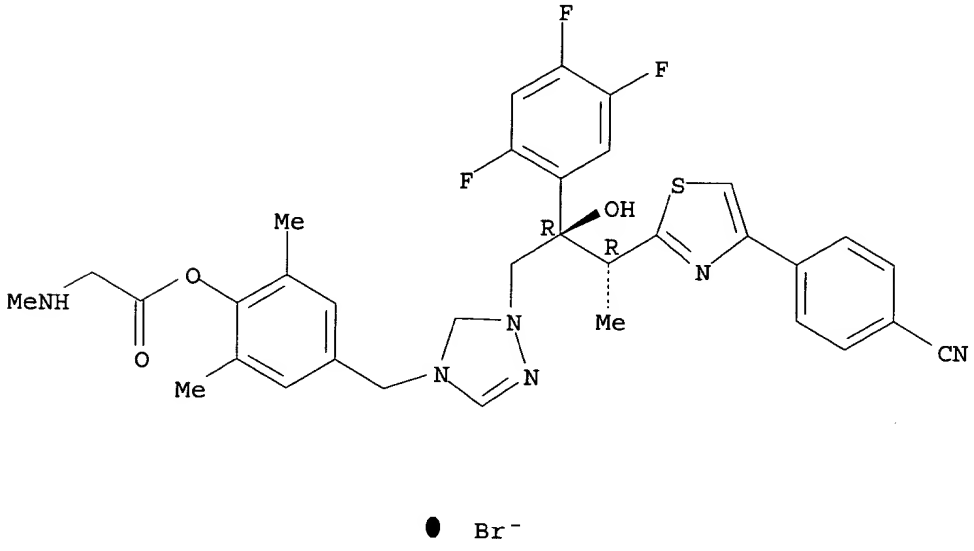
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 241479-36-7 USPATFULL
CN Glycine, N-methyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-hydroxy-2-(2,4,5-trifluorophenyl)butyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Br^-

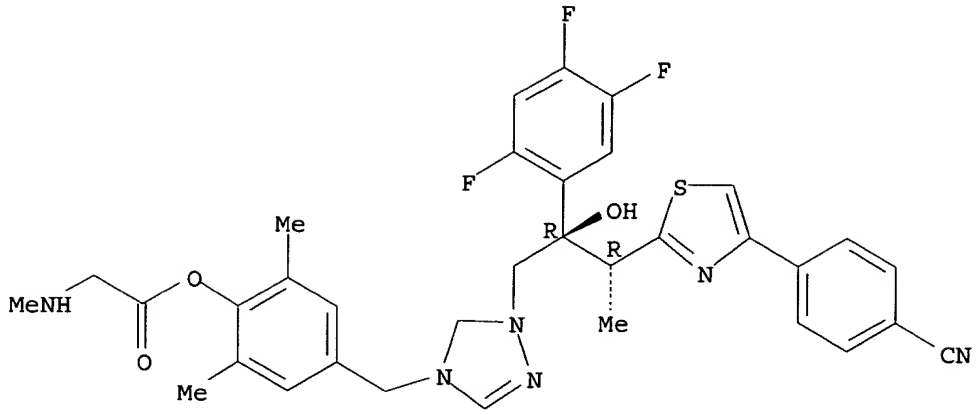
FRAGMENT DIAGRAM IS INCOMPLETE

RN 241479-38-9 USPATFULL
CN Glycine, N-methyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-hydroxy-2-(2,4,5-trifluorophenyl)butyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 241479-37-8
CMF C34 H32 F3 N6 O3 S

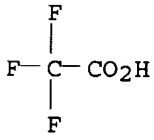
Absolute stereochemistry.



FRAGMENT DIAGRAM IS INCOMPLETE

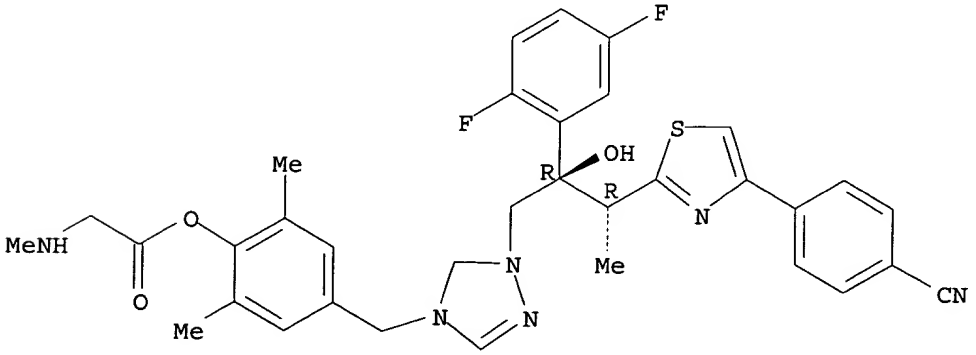
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 241479-39-0 USPATFULL
CN Glycine, N-methyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Br^-

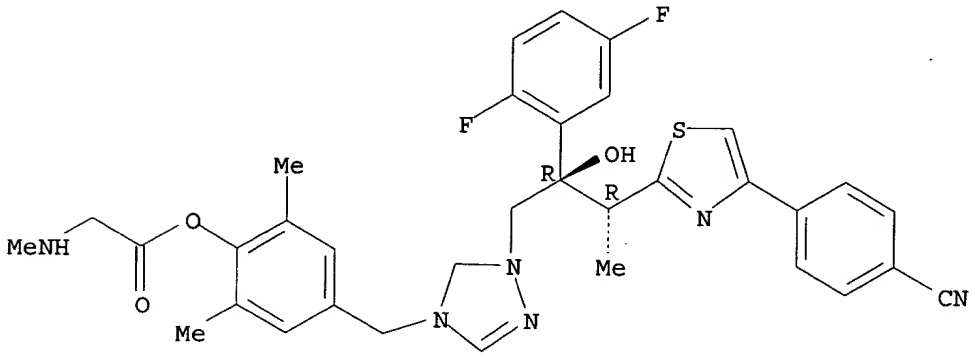
FRAGMENT DIAGRAM IS INCOMPLETE

RN 241479-41-4 USPATFULL
CN Glycine, N-methyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 241479-40-3
CMF C34 H33 F2 N6 O3 S

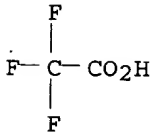
Absolute stereochemistry.



FRAGMENT DIAGRAM IS INCOMPLETE

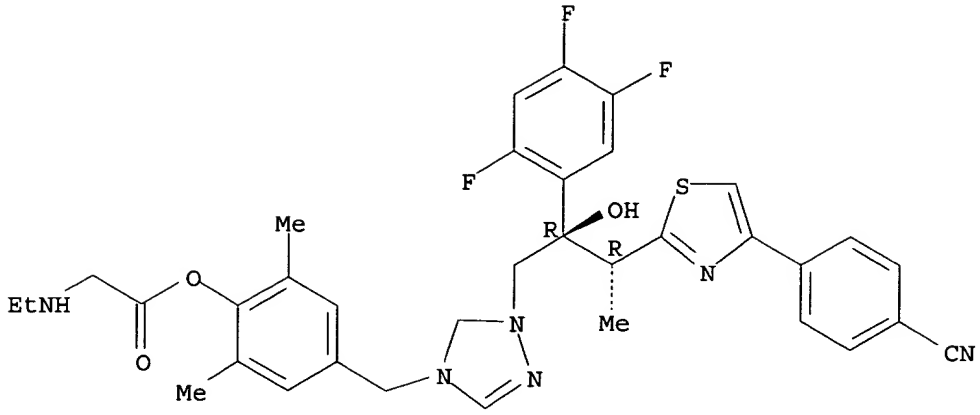
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 241479-45-8 USPATFULL
CN Glycine, N-ethyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-hydroxy-2-(2,4,5-trifluorophenyl)butyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Br^-

FRAGMENT DIAGRAM IS INCOMPLETE

RN 241479-47-0 USPATFULL

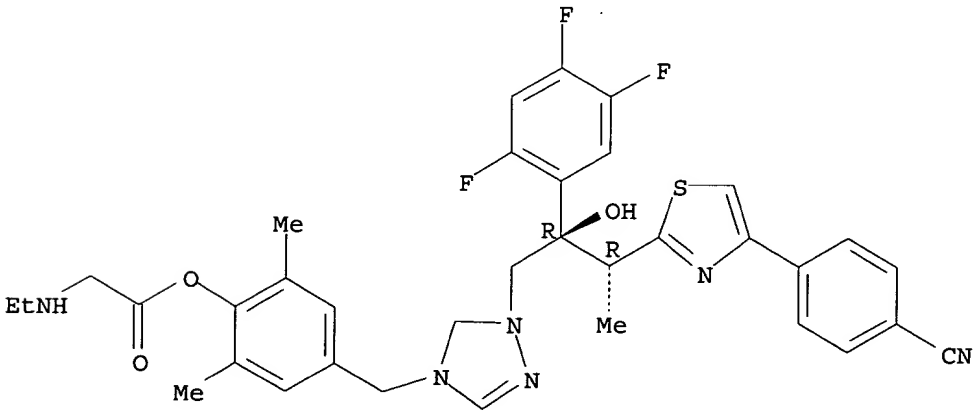
CN Glycine, N-ethyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-hydroxy-2-(2,4,5-trifluorophenyl)butyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 241479-46-9

CMF C35 H34 F3 N6 O3 S

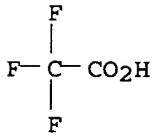
Absolute stereochemistry.



FRAGMENT DIAGRAM IS INCOMPLETE

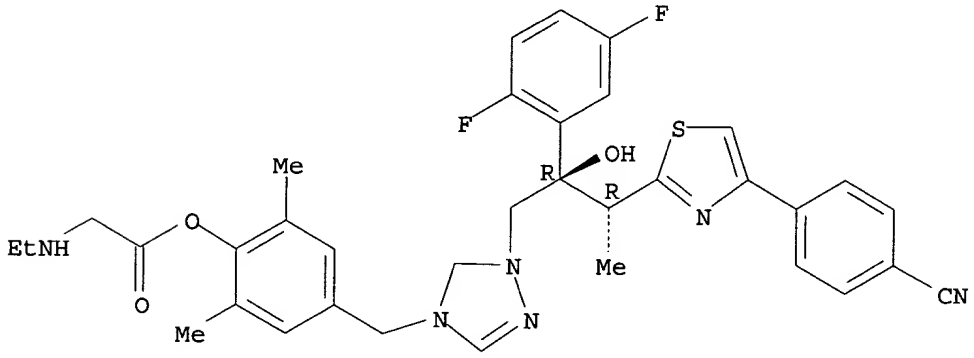
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 241479-48-1 USPATFULL
CN Glycine, N-ethyl-,
4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Br^-

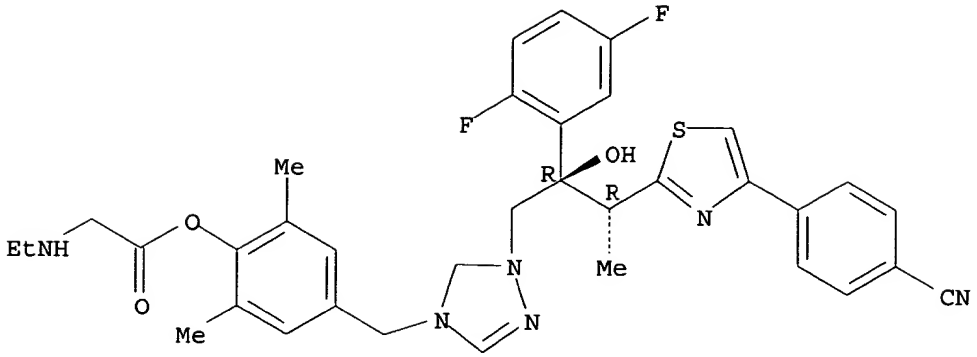
FRAGMENT DIAGRAM IS INCOMPLETE

RN 241479-50-5 USPATFULL
CN Glycine, N-ethyl-,
4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 241479-49-2
CMF C35 H35 F2 N6 O3 S

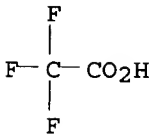
Absolute stereochemistry.



FRAGMENT DIAGRAM IS INCOMPLETE

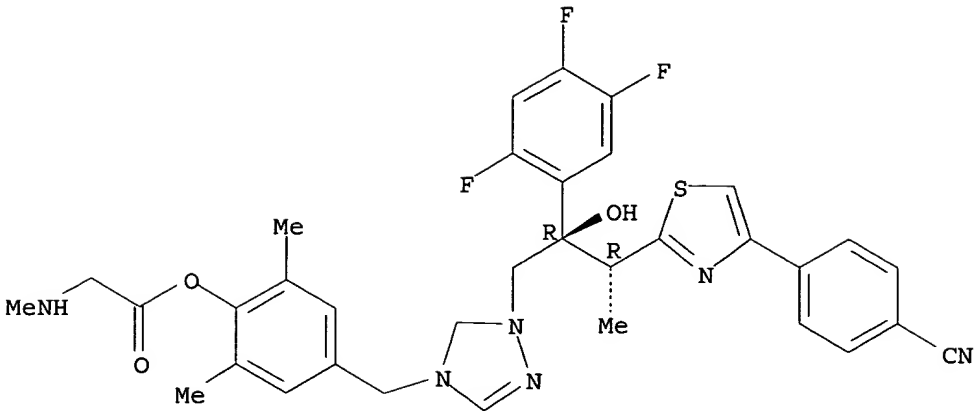
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 241479-54-9 USPATFULL
CN Glycine, N-methyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-hydroxy-2-(2,4,5-trifluorophenyl)butyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, chloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Cl⁻

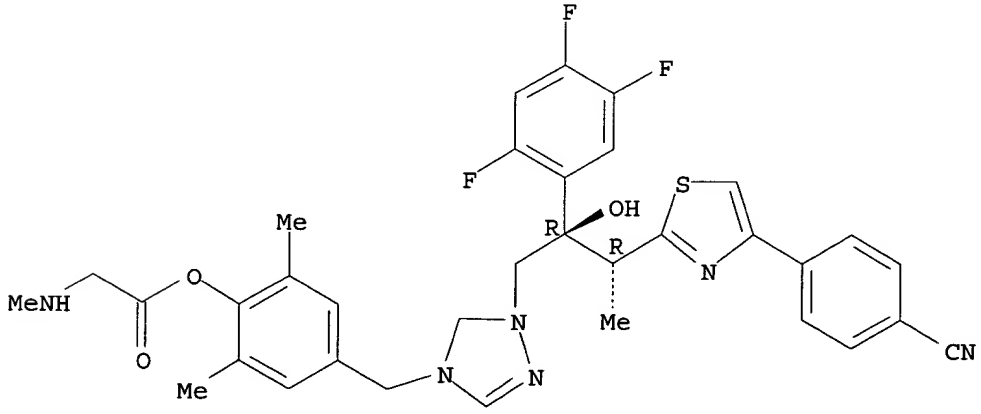
FRAGMENT DIAGRAM IS INCOMPLETE

RN 241479-55-0 USPATFULL

CN Glycine, N-methyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-hydroxy-2-(2,4,5-trifluorophenyl)butyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, chloride, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



● Cl⁻

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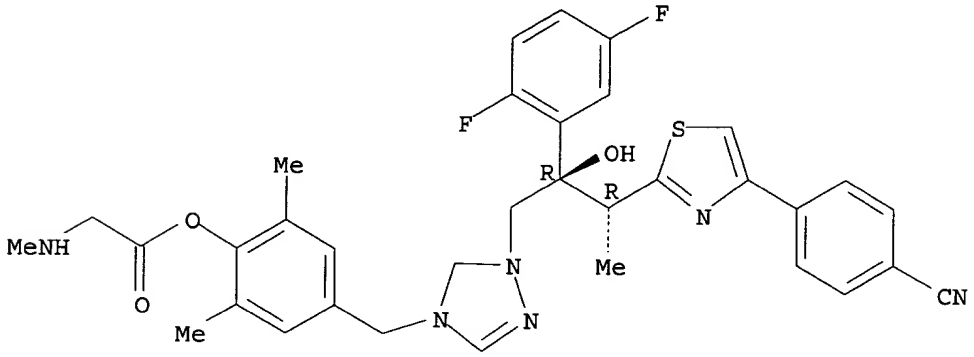
● HCl

FRAGMENT DIAGRAM IS INCOMPLETE

RN 241479-56-1 USPATFULL

CN Glycine, N-methyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, chloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Cl^-

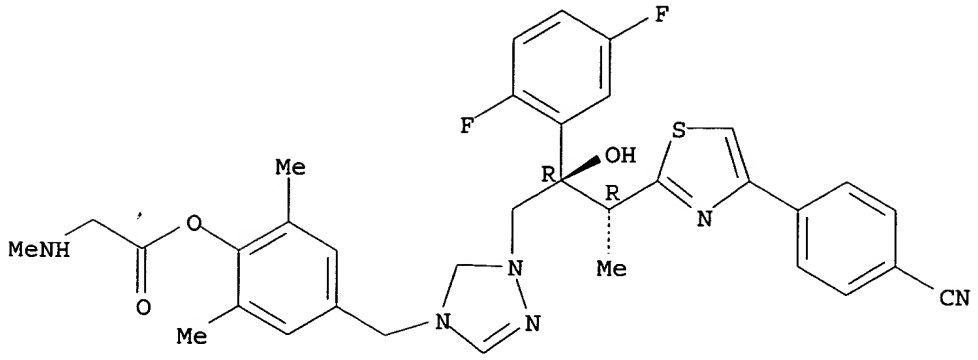
FRAGMENT DIAGRAM IS INCOMPLETE

RN 241479-57-2 USPATFULL

CN Glycine, N-methyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, chloride, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



● Cl^-

PAGE 2-A

● HCl

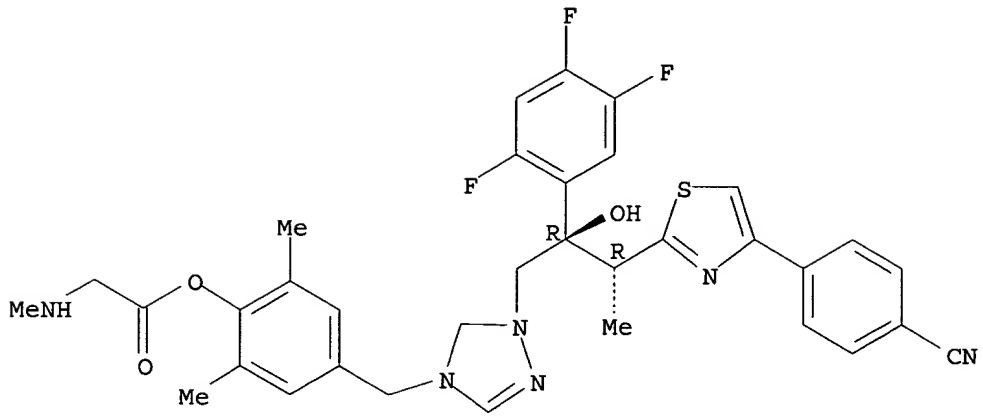
FRAGMENT DIAGRAM IS INCOMPLETE

RN 241479-60-7 USPATFULL

CN Glycine, N-methyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-hydroxy-2-(2,4,5-trifluorophenyl)butyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide, monohydrobromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



● Br^-

PAGE 2-A

● HBr

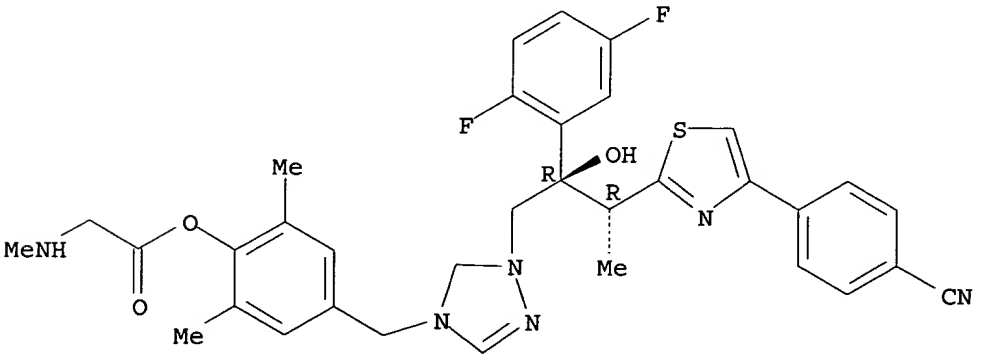
FRAGMENT DIAGRAM IS INCOMPLETE

RN 241479-61-8 USPATFULL

CN Glycine, N-methyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide, monohydrobromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



● Br^-

PAGE 2-A

● HBr

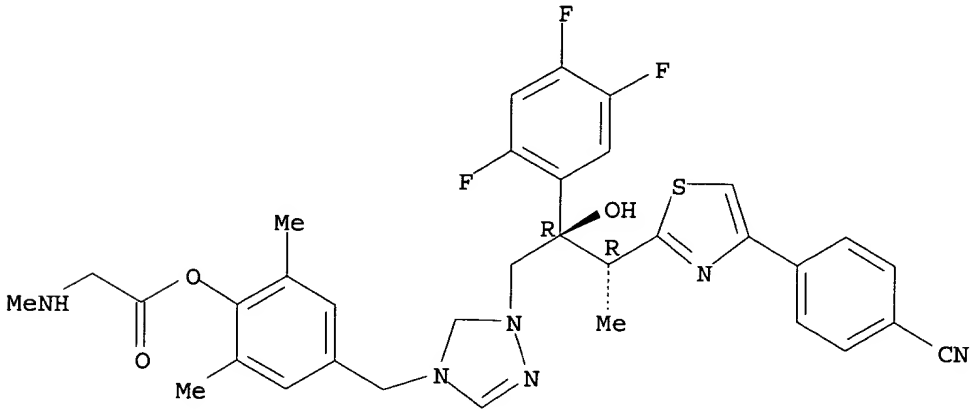
FRAGMENT DIAGRAM IS INCOMPLETE

RN 241479-63-0 USPATFULL

CN Glycine, N-methyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-hydroxy-2-(2,4,5-trifluorophenyl)butyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



● Br^-

PAGE 2-A

● HCl

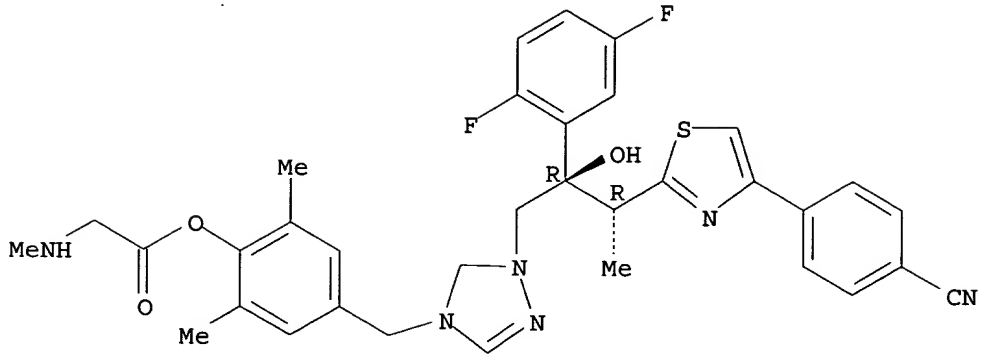
FRAGMENT DIAGRAM IS INCOMPLETE

RN 241479-64-1 USPATFULL

CN Glycine, N-methyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



● Br^-

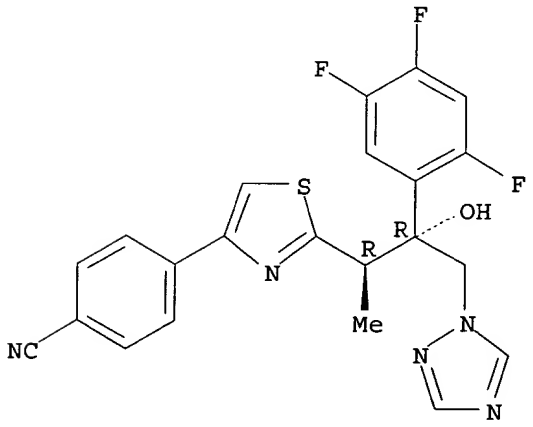
PAGE 2-A

● HCl

FRAGMENT DIAGRAM IS INCOMPLETE

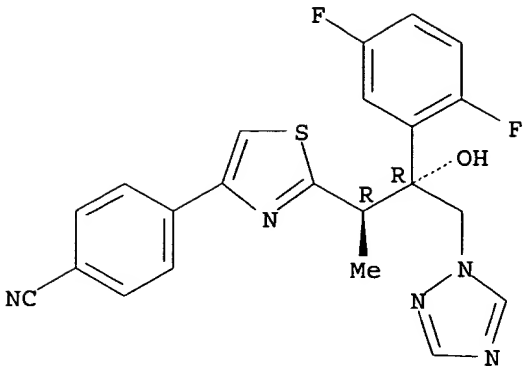
RN 241479-66-3 USPATFULL
CN Benzonitrile,
4-[2-[(1R,2R)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)-2-(2,4,5-trifluorophenyl)propyl]-4-thiazolyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 241479-67-4 USPATFULL
CN Benzonitrile, 4-[2-[(1R,2R)-2-(2,5-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-4-thiazolyl]- (9CI) (CA INDEX NAME)

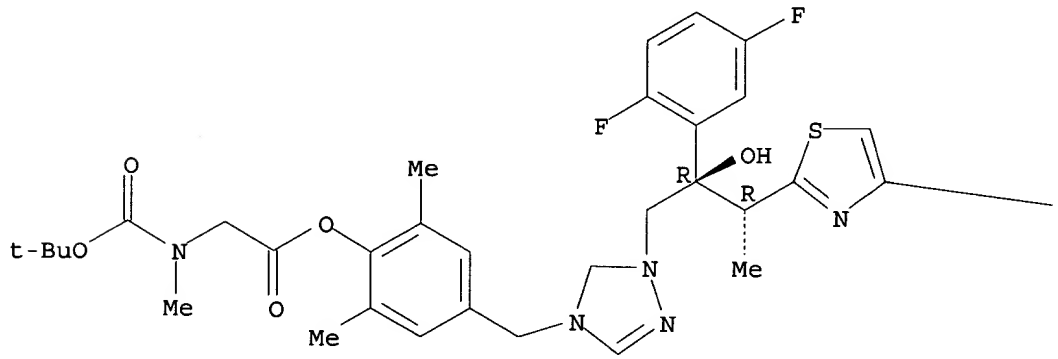
Absolute stereochemistry.



IT **241479-83-4P 241479-87-8P**
(prepn. of cyanophenylthiazolyltriazolylbutanols as antifungals)
RN 241479-83-4 USPATFULL
CN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-N-methyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide (9CI) (CA INDEX NAME)

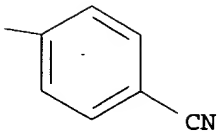
Absolute stereochemistry.

PAGE 1-A



● Br^-

PAGE 1-B



FRAGMENT DIAGRAM IS INCOMPLETE

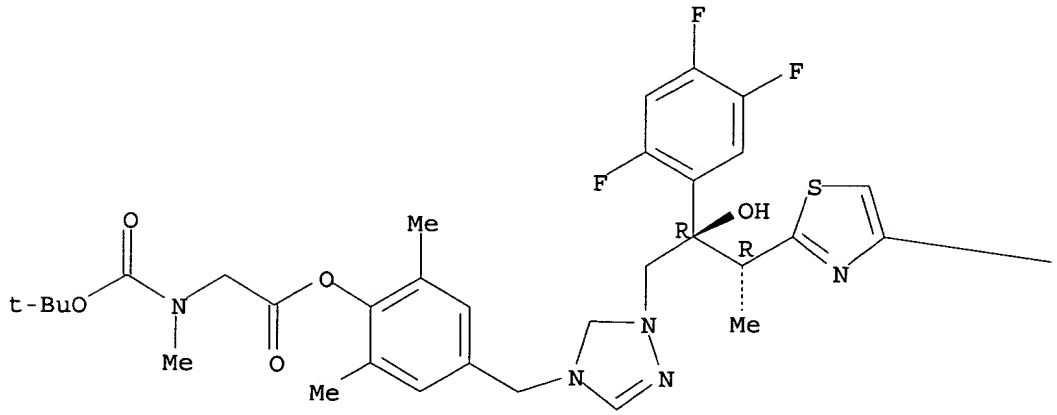
RN 241479-87-8 USPATFULL

CN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-N-methyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-hydroxy-2-(2,4,5-trifluorophenyl)butyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide (9CI)

(CA INDEX NAME)

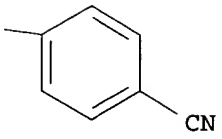
Absolute stereochemistry.

PAGE 1-A



● Br^-

PAGE 1-B



FRAGMENT DIAGRAM IS INCOMPLETE